Evolution of Off-phase Variants in the L1_2 Type Ordering(Session IV : Structures & Patterns, The 1st Tohwa University International Meeting on Statistical Physics Theories, Experiments and Computer Simulations)

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The method of time-dependent Ginsburg-Landau (TDGL) theory[1] has been extensively used to account for the general characteristics in the evolution of ordered domain structure and the behaviors of antiphase boundaries in the course of thermal treatment of binary alloys, which order in B2 or DO_3 structure, for example, CuZn, FeCo and Fe_3Al.[2,3] The theory has also been extended to include the case of phase separation induced by ordering as a dynamical problem of coupling between the conserving variable of local composition $c(r,t)$ and the nonconserving one of local degree of order $s(r,t)$.[3,4] In the case of Fe_3Al and Fe-Ga system two types or ordered structures are involved, and the phenomenological theory has been successfully attempted to include two independent order parameters besides the local alloy composition.[5] It is to be noted here that in these order-disorder transformations the transitions were of the second order, and the coexistence of A2 (disorder) and B2 or DO_3 in the same sample, does not necessarily mean the first order transition. It is known that the system such as Cu_3Au forms the so-called $L1_2$ ordered structure, which is of the first order transition.

In the present work a simple theory is unfolded to describe the development of off-phase variants in the $L1_2$ type ordering in binary alloys such as Cu_3Au. In this type of order there are four different crystallographic variants, anyone of which is displaced from the other three by one of the three primitive basic translations of an fcc structure. In the present model the fcc lattice is decomposed into four simple cubic sublattices, where the atomic arrangement in the long range order is represented by three independent order parameters. Each one of these parameters has a definite physical meaning, in the sense that it is related to the corresponding structure factor for a superlattice reflection. The state of order of the atomic arrangement in the system is defined by a point in the three dimensional Euclid space spanned by these three order parameters. The actual $L1_2$

order structure is given by anyone of the four tips of a regular tetrahedron around the origin, which represents the disordered state. A simple free energy of the Landau type is introduced as a function of these order parameters up to their fourth powers. It is shown that the free energy includes two parameters depending on the temperature, and the equilibrium value for the $L1_2$ order parameter is determined by them as a function of the temperature. Below the critical temperature the disordered state gives a maximum of the free energy, and is unstable against ordering. Small disturbances in the atomic arrangement cause the system to change their state of order following a path in the order space, and to fall into one of the four minimum points of the free energy, which are the corners of the tetrahedron in that space. In order to investigate the dynamical behavior of the ordering, the surface and the interfacial energies are introduced, between the ordered phase and the disordered one, or between any pair of the ordered variants. The equations of motion for the space-time evolution of the order state are derived by the TDGL (time dependent Ginsburg-Landau) method. To emphasize the reasonableness of our approach, the theory is reduced to a two-dimensional case with two order parameters with three equivalent minimum points of the free energy, which form a regular triangle, with the maximum point at the center. The PC simulation for the pattern formation of ordering with multiple variants is performed on a square matrix, and some results of interest were obtained. Implications of the present method as applied to the other types of ordered structure are to be mentioned together with its applications.

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